Fundamentals of Combustion
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Lecture – 07
Stoichiometry - Part 2 Worked Examples

So, let us see the worked example for the content what we covered. So, we are going to go through what is called Stoichiometry worked examples now.

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So, the first example the problem and the solution is given here, I will just try to explain this. So ethanol, C_2H_5OH is burnt in a furnace with an equivalence ratio of 1.1.

So, it is a rich mixture, where more fuel than air is supplied. The condition given is, if no hydrogen or oxygen is found in the exhaust. Determine the product composition per kilomole of fuel.

So, that is the problem we have given here. See the ethanol reaction is given here in this, say ethanol C_2H_5OH, when you write this stoichiometric reaction.

$$C_2H_5OH + 3(O_2 + 3.76\ N_2) \rightarrow 3H_2O + 2CO_2 + 11.28N_2$$
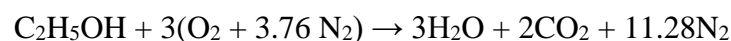
So, you know that you have to assume a complete combustion. So, all the H is converted into H_2O. There are 6 H atoms. So, $3H_2O$ is formed and C_2 is converted into $2CO_2$.

So, this is the stoichiometric reaction and but the given data is the equivalence ratio is 1.1; that means, you are not supplying the stoichiometric air the air supplied is 3 by 1.1. So, this is actually 3 by phi.

$$C_2H_5OH + (3/1.1)(O_2 + 3.76\ N_2) \rightarrow 3H_2O + aCO_2 + bCO + 10.2545N_2$$
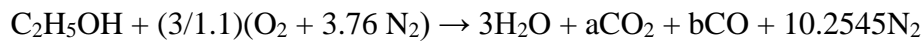
So, that is the amount of air which is supplied. So, you can see that if phi is less than 1, you will supply more air than the stoichiometric quantity. Now, in this case since phi is 1.1 that is greater than 1, you get fuel rich mixture. Now, for this the condition given is there is no hydrogen left, this is correct.

Because, obviously, what happens is hydrogen is a very fast reactive fuel. So, it first consumes all the oxygen, then remaining oxygen is actually available for oxidising the C. So, that means, there will be no oxygen left. So, if the engine exhaust has no hydrogen or oxygen left. What you should write as here? You will follow all the H_2O. So, for example, in stoichiometry condition, you see that for 1 mole of ethanol 3 moles of H_2O are formed.

Similarly, in this rich combustion also first hydrogen is fully consumed or it takes all the oxygen required for its oxidation. So, 3 moles of H_2O is formed first. But, now you can see that for C for C_2 to oxidise oxygen is not enough.

So, what happens is? Some amount of CO_2 is formed and some amount of CO is formed, because the oxygen is not available see 3 moles of oxygen is required for combustion, but you are supplying 3/1.1 that is less than 3 for the actual mixture.

So, you will get some amount of carbon monoxide in the mixture. Now, you have equations in terms of atom balance. Hydrogen balance does not appear here, because its already balanced, but let us take carbon balance 2 carbon atom in the left hand side a plus b are the carbon atoms in the right hand side. So, just add them. So, you get one equation involving a and b.

Similarly, do O balance in the left hand side you will see that the fuel has half O molecule that is half of the O molecule here, plus 3/1.11 in the oxidizer.

Left hand side you have half plus 3/1.1 kilomoles of oxygen, right hand side $3H_2O$ has $3/2\ O_2$. So, $3/2\ O_2$ corresponding to H_2O, then 'a' CO_2 will have 'a' moles of oxygen and 'b' CO will have $b/2\ O_2$.

So, now if you balance this and you will get another equation involving a and b. So, solving these two together you will get a = 1.4546 and b = 0.5454. So, what is asked is the product composition per kilomole of fuel.

So, you have already written the equation for 1 kilomole of fuel here. So, the product formed are 3 H_2O + 1.4546 CO_2 + 0.5454 CO and 10.2545 N_2. So, these are the number of kilomoles of products which are formed.

So, please understand here that if there is a rich combustion and some conditions are given like in general practice, we can take that all the hydrogen is consumed. But, let us take a example, for example, if this equivalence ratio is more than 1.1 say, it is 1.5 then what happens is even hydrogen may not have enough oxygen to combust.

So, in that case you will see hydrogen remaining in the product. For example, H_2 will be there. So, you have to include that also, but in this case since the exhaust is measured and it has no hydrogen or oxygen, we can write like this.

Now, the point when I say no hydrogen is given, I understand that all the hydrogen is consumed. So, it is transformed to water vapour. But what is the point writing no oxygen because, already it is oxygen starved correct.

So, we do not have enough oxygen here. So obviously, there should be no oxygen coming out of the exhaust. But the point why we are given here no oxygen is because, you can understand that if temperature is high enough then products can dissociate.

For example, CO_2 can dissociate to form CO and O_2. So, that dissociation product O_2 can come out, but in this case the temperatures are not so high. When the combustion takes place within the furnace. So, what happens is, there is no oxygen available due to dissociation.

There is no oxygen available for complete combustion of carbon, as well as there is no oxygen available due to dissociation. So, this is the problem where you try to do this, stoichiometric analysis of a rich mixture of ethanol and air.

The second problem, in a combustion process with decane, that is decane is straight chain alkene $C_{10}H_{22}$. C_nH_{2n+2}. So, $C_{10}H_{22}$ and air, air is the oxidizer, it is burnt and the products are analysed using a volumetric analyser. For example, Orsat analyser is a typical example for a volumetric analyser, which measures the product composition.

This Orsat analyser normally when you let in the exhaust gas into this Orsat analyser first of all you have to filter out the water vapour. So, condense the water and filter out the liquid water then the other gases are fed; that means, you are measuring only the dry mole fractions.

So, such an analysis presents 83.61% of nitrogen, then 4.91% of O_2 and 10.56% of CO_2 and you can see that there is some quantity of CO also. So, here O_2 is also present and CO is also present.

So, that is what I told you in the previous problem that O_2 maybe there; obviously, this may be a problem where O_2 oxygen is supplied in excess than required for the complete combustion; However, due to some dissociation CO is formed.

Now for this scenario, you do not know anything else it is a dry product, we do not even know the mole percentage. We know that product mole fractions are given, because the volumetric fractions are nothing, but mole fractions.

You know the mole fractions in this dry basis, there is no water vapor involved. But obviously, you know that when a hydrocarbon burns it will produce water vapor.

But the water vapor has been condensed and the liquid is removed. The composition of other gases is presented in this list. Now, what we required to find is the equivalence

ratio, then percent theoretical air of the reactants, and the molecular weight of products mole fraction of CO_2 these all we want.

Now if we add up this dry fractions you know see for example, 83.61 N_2 + 4.91 O_2 + 10.56 CO_2 + 0.92 CO, you will see that they sum up to 100 kilomoles or 100%.

Let us assume that 100 kilomoles of dry products are formed. In 100 kilomoles of dry products, we have 83.61 kilomoles of nitrogen 4.91 kilomoles of oxygen 10.56 kilomoles of CO_2 and 0.92 kilomoles of CO.

Let us assume that these are the products. What I am trying to do here is change the percentage into kilomoles. So, to obtain this much kilomoles of dry products excluding the water which is formed, how much fuel I have to burn.

Let us assume that I burn x kilomoles of fuel, you can also assume some kgs. So, here I am assuming x kilomoles of decane is burnt to produce, 100 kilomoles of dry products as given in the problem.

$$x \, C_{10}H_{22} + a \, (O_2 + 3.76 \, N_2) \rightarrow b \, H_2O + 10.56 CO_2 + 0.92 CO + 83.61 N_2 + 4.91 O_2$$
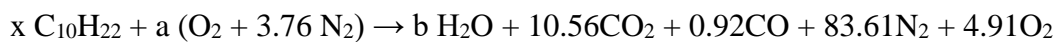
If I do that then I can write the chemical equation as x moles of $C_{10}H_2$ here $C_{10}H_{22}$ plus, I do not know how much amount of oxidizer is required or number of moles of oxygen. So, 'a' times the air, air is O_2 + 3.76 N_2 giving I do not know again the number of moles of H_2O formed, because this is only dry basis on dry basis only we have got the other product composition.

Let us assume 'b' kilomoles of H_2O is formed along with whatever is given here, so, CO_2 10.56 kilomoles of CO_2 then 0.92 kilomoles of CO and 4.91 kilomoles of O_2 and 83.61 kilomoles of N_2. These are all the dry products. The percentage I have converted into this.

To achieve this dry products composition in terms of kilomole I have to burn x kilomoles of fuel and with 'a' kilomoles of a × 4.76 kilomoles of air and in this way 'b' kilomoles of H_2O is formed. But then I can see that straightaway I cannot get the value of 'b', because 22x = b so, first I have to get the value of x.

Now let us do the atom balances for this equation. So, by N balance straightaway, we can see that a × 3.76 will give you the N, 83.61. So, you will get directly the value of 'a' so, that is the amount of oxidizer supplied. So, number of kilomoles of air is 22.2367 × 4.76 kilomoles of air is supplied.

Now, do the C balance because you know CO and CO_2's number of moles in the products are known. So, 10 x in the left-hand side will be equal to 10.56 + 0.92. So, you

will get the value of x so; that means, instead of just burning 1 kilomole of fuel, I am burning 1.148 approximately 1.15 kilomoles of decane.

So, the fuel is slightly higher than 1, 1 kilomole. So, its 1.15, now do the H balance to get the value of 'b' that is $22 \times x$, now value of x is known. So, 22×1.148 will be equal to in the right-hand side 2b, this is number of H atoms. So, b = 12.628.

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So, the unknowns are x, a and b we have got that. Now we will try to write the equation you did not even do that, but I am trying to do this. For example, normally its our practice that you can see this in the previous examples also, here it is our practice to write the equation in 1 kilomole of fuel. So, taking 1 kilomole of fuel we are writing the equation.

But, in this case we have taken x kilomoles of fuel. So, now, try to divide this by x. So, you get the equation. Now, after evaluating x, a and b which are unknowns we are trying to write the equation in terms of 1 kilomole of fuel. So, now, dividing throughout by x I am writing this equation like this.

Now, see the number of kilomoles of oxygen is 19.37. So, you find the actual air fuel ratio which is nothing, but 19.37 times 4.76 number of moles in the air, which is 1 plus 3.76, into molecular weight of air. So, this is the number of moles of oxidizer into this is the number of moles of air then this is the molecular weight of air.

So, now divided by the molecular weight of fuel which is $(10 \times 12) + 22$ so, 120 plus 22 this is the molecular weight of $C_{10}H_{22}$. Now it will be 18.726; obviously, we know that approximately 15 kilo kilogram of air is required to burn 1 kg of higher order hydrocarbons like $C_{10}H_{22}$.So, actually the actual stoichiometric air fuel ratio is so, you

know 'a', 'a' is x + (y / 4). So, x = 10, y = 22 so, 'a' will be (x + y / 4), this into 4.76 × 28.84 / 142 will be stoichiometric air fuel ratio, you get around 15. But you are supplying more than this. So, the equivalence ratio is less than 1, because the actual air supplied is higher than the stoichiometric air.

So, equivalence ratio, this is stoichiometric air fuel ratio divided by actual air fuel ratio. That is the definition of equivalence ratio, so you will get 0.8.

Even if you are supplying excess air due to dissociation, you find that CO is formed in small amount, little amount of CO is formed in the products, because of dissociation.

Now what is asked? So, equivalence ratio is got then percent theoretical air is 100 by phi so, 100 / 0.8 so, 125 percent. Then you want the molecular weight of the products and the mole fraction of CO_2.

Total number of moles you can find here just add this, 11 + 9.1986 + 0.801 + 72.83 + 4.277 that is 98.81 kilomoles. The mole fraction of CO_2 is number of kilomoles of CO_2 that is 9.1986 divided by 98.1 that will be this.

Similarly, you calculate the molecular weight of the products is nothing, but $\sum X_i$ that is mole fraction of each product species multiply it by its own molecular weight so, $\sum X_i M_i$. Now, you can write this as n_i.

So, n_i is 11, 9.1986… etcetera into M_i divided by n_{total}. So, we will get the molecular weight as this. This is very close to nitrogen molecular weight because nitrogen's number of moles are very high, mole fraction is very high for nitrogen.

You can see that in this case by just knowing the dry composition of the products we can find the amount of air supplied. The amount of air supplied can be obtained and so, the product analysis is very very important.

So, by this product analysis we are able to get the this. We can also determine how much water base formed by this. Once you know the fuel composition, we can find how much air has been supplied to get this product and so on. Its a simple stoichiometric calculation.

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Worked Example 3

(3) A typical fuel gas mixture has the following volumetric analysis 10% CO, 45% H_2, 35% CH_4, 4% C_2H_2, 2% O_2, 2% N_2 and 2% CO_2. Determine the stoichiometric air-fuel ratio. Also determine the product composition when this is burnt in 20% excess air.

Solution: Stoichiometric equation for this mixture is written as,

$0.1CO + 0.45H_2 + 0.35CH_4 + 0.04C_2H_2 + 0.02(O_2 + N_2 + CO_2)$ } fuel mixture
$+ a(O_2 + 3.76\ N_2) \rightarrow bH_2O + (c + 0.02)CO_2 + (3.76a + 0.02)N_2$

C balance: $0.1 + 0.35 + 0.08 + 0.02 = c + 0.02 \Longrightarrow$ $c = 0.53$
H balance: $0.45 + 0.7 + 0.04 =$ $b = 1.19$
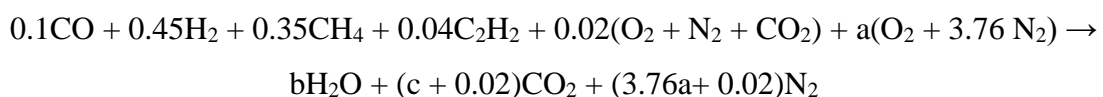O balance: $0.1/2 + 0.02 + a = b/2 + c + 0.02 \Longrightarrow$ $a = 1.075$

$0.1CO + 0.45H_2 + 0.35CH_4 + 0.04C_2H_2 + 0.02(O_2 + N_2 + CO_2)$
$+ 1.075(O_2 + 3.76\ N_2) \rightarrow 1.19H_2O + 0.55CO_2 + 4.062N_2$

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So, let us see the worked example 3, now we will consider a fuel mixture, which consists of by volume 10% CO, 45% H_2, 35% CH_4, 4% C_2H_2 and some oxygen 2% O_2 and N_2 and CO_2 are also present.

Now, what is required is we have to find the stoichiometric air fuel ratio and product composition, when this fuel mixture is burnt with 20 percent of excess air. That is the requirement.

Now, let us consider 1 kilomole of fuel as per the volumetric analysis. The mole fractions which is given here actually the volumetric fractions are mole fractions so, we will just divide it by 100. So, that you will get mole fraction, when you add it, it will be 1.

$$0.1CO + 0.45H_2 + 0.35CH_4 + 0.04C_2H_2 + 0.02(O_2 + N_2 + CO_2) + a(O_2 + 3.76\ N_2) \rightarrow$$
$$bH_2O + (c + 0.02)CO_2 + (3.76a + 0.02)N_2$$

So, 1 kilomole of fuel mixture we will take which consists of say, 10 / 100, 0.1 CO, then 45 / 100, 0.45 H_2 and 35 / 100, 0.35 CH_4, then 4 percent C_2H_2, 0.04 C_2H_2 and 2 percent oxygen, nitrogen and CO so, 0.02 times these 3.

Now, oxygen we do not know much moles of oxygen to be added. So, let us say 'a' moles of oxygen is added to form 'b' moles of H_2 'c' moles of CO_2 due to combustion plus already 0.02 kilomoles of CO_2 is present in the reactant mixture.

So, that will also translate here so, c plus 0.02 CO_2. Similarly, nitrogen in the oxidizer stream is 3.76 times 'a' plus what is present in the fuel stream is 0.02N_2 so, 0.02. So, that will add up.

Now, the oxygen in the fuel and the oxygen in the oxidizer stream both will be used to completely burn the fuel components in the fuel mixture. So, like we did for ethanol the O in the ethanol was utilised for burning complete combustion.

So, we supplied only lesser air. Similarly, since fuel itself has some inherent air, we supply only air excluding that part. So, this will be the fuel mixture.

Now, do the C balance 0.1 CO so, 0.1 here then 0.35 then 0.04 into 2 that is 0.08 in the left-hand side, plus CO_2 has 0.02. So, that is the current balance right hand side you have c plus 0.02 so, solving which you get c equal to 0.53. Now, H balance H_2 is say 0.45 here. So, I am writing 0.45 then CH_4. 4 CH_4 is there so, 0.35 into 2 is 0.7 plus here C_2H_2.

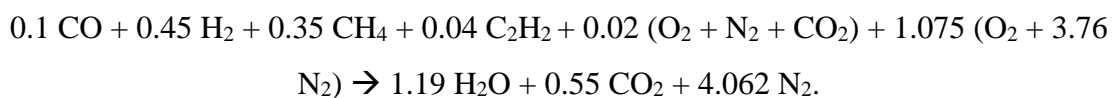$$\text{C balance: } 0.1 + 0.35 + 0.08 + 0.02 = c + 0.02 \rightarrow c = 0.53$$

$$\text{H balance: } 0.45 + 0.7 + 0.04 = b = 1.19$$

$$\text{O balance: } 0.1/2 + 0.02 + a = b/2 + c + 0.02 \rightarrow a = 1.075$$

So, that there H_2 is there. So, 0.04 here, left hand side these are the H_2's and the right-hand side 'b' so, solving which you get 'b' as 1.19. Similarly, O balance, O balance is 0.1 into O_2 0.1 divided by 2 times O_2 plus here 0.02 O_2. So, 0.02 give plus 'a' aO_2 in the left-hand side, reactant side, product side 'b' by 2 O_2 for the hydrogen, then c plus 0.02 O_2 here that is all.

Now if you solve for 'a', see you know 'b' value and 'c' value from the C and H balances. So, calculate 'a'.

That will be stoichiometric reaction,

$$0.1\ CO + 0.45\ H_2 + 0.35\ CH_4 + 0.04\ C_2H_2 + 0.02\ (O_2 + N_2 + CO_2) + 1.075\ (O_2 + 3.76\ N_2) \rightarrow 1.19\ H_2O + 0.55\ CO_2 + 4.062\ N_2.$$

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So, this is the stoichiometric equation. So, continuing the example for the fuel mixture you can see that the amount of oxidizer required is 1.075 and these are the composition of the products which have been measured. Please understand the stoichiometric reaction if you do not have any oxygen leftover in the fuel so, that is the way you write this.

Now the molecular weight of fuel is calculated, because the mole fractions are known we can calculate the molecular weight of the fuel mixture and you can see that is 12.42. So, here this 104 is nothing, but $32 + 28 + 44$ which are these three. Now, you do this and the molecular weight is very low kg per kilomole.

Because, you can see that the 45% of hydrogen and 35% of methane, which have lower molecular weight these compounds are present. So, the overall molecular weight has reduced to 12.42. Now, stoichiometric air fuel ratio is $1.075 \times 4.76 \times 28.84 / 12.42$. So that will be 11.882 kilo gram per kilogram of fuel.

Now, what is asked is when it is so, this is the stoichiometric air fuel ratio that is the first one what we have to determine. Second one is when the fuel mixture is burnt in 20% excess air. So, how will you do this, same fuel mixture plus 1.07 times into 1.2. So, 20% excess air you see that there is some oxygen present in the product.

The complete combustion, like in stoichiometric mixture, complete combustion takes place. So, the number of moles of H_2O is 1.19, number of moles of CO_2 is 0.55 and N_2.
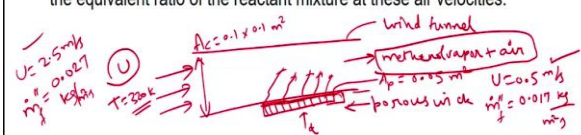
So, this will be the composition of the product. So, we want composition of the products when 1 kilomole of fuel mixture is burnt. So, that is this, so, this is the composition of products.

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Now, let us consider problem where methanol is used and it is evaporated through a porous wick. So, in an atmospheric pressure pre vaporizer a horizontal porous wick saturated with methanol is kept in flush with the bottom wall of a horizontal wind tunnel. So, this is the porous wick horizontal porous wick. This is kept in the in flush with the bottom wall of the wind tunnel. This porous block is kept in flush air flows at a given velocity over surface. So, air comes here like this and flows over the surface of the wick.

It has some velocity and temperature is 320 Kelvin. So, that is kept constant and the velocity is varied and it is actually supplied like this. Now, as a result, because this is at 320 Kelvin higher temperature than the ambient, methanol vaporizes, and please understand that this wick is saturated with methanol.

So, always methanol is supplied to the wick and it is always saturated with methanol. So, as the methanol vaporizes more and more liquid methanol will come and saturate the wick. That is the problem so, it's a steady evaporation problem.

When you vary the 'U' you will get more evaporation and so on. So, air flows at a given velocity over the surface of the wick at a temperature of 320 Kelvin as a result methanol vaporizes and mixes with air.

So, here we get methanol vapor plus air, premixed methanol vapor and air, so this is called pre vaporizer. I tried to vaporize the fuel and premix it with air and send it to the combustion chamber. So, maybe combustion chamber is next to the wind tunnel. Now, reactant mixture flows out of the wind tunnel into the combustion chamber. The cross section of the wind tunnel is 0.1 metre by 0.1 metre.

The cross section of this wind tunnel is 0.1 by 0.1 metre square. A_P is the surface area of the porous plate. So, A_P will be 0.05 metre square. Now, at an air velocity of 0.5 metre per second, when 'U' equal to 0.5 metre per second.

The evaporation rate per unit area of the porous plate, the fuel is vaporizing from this the evaporation per unit area is so, we will say mass evaporation rate per unit area of methanol fuel is 0.017 kg per metre square second. Now, when the air velocity is increased to 2.5 metre per second so, when 'U' equal to 2.5 metre per second, the evaporation rate increases to 0.027 kg per metre square second.

So, that is the evaporation rate of the fuel is now 0.027 kg per metre square second. So, kg per second per metre square that is the evaporative flux. Now, determine the equivalence ratio of the reactant mixture at these velocities. Now, the evaporation takes place. What is the equivalence ratio of the mixture?

Methanol vapor and air comes out of the wind tunnel and goes into the combustion chamber, what is the equivalence ratio of these two velocities 0.5 metre per second and 2.5 metre per second. Now this is the problem.